

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 251 °C

Global applicability domain: Inside

Local applicability domain index: 4.59e-01

Confidence level: 3.77e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chloranil</div> <div>Measured: 290</div> <div>Predicted: 251</div>	<div>Image not found</div> <div>Bromanyl</div> <div>Measured: 293</div> <div>Predicted: 280</div>	<div>Image not found</div> <div>Heptachlor</div> <div>Measured: 95.5</div> <div>Predicted: 97.7</div>
<div>Image not found</div> <div>MCPA-thioethyl</div> <div>Measured: 41.5</div> <div>Predicted: 46.5</div>		